Tetrachloroethylene-13C1 287399-46-6 | DTXSID30481626

Mod	el P	erfor	man	e:
14100	O 1	01101	HILLIN	\mathcal{I}

Model	Data

Weighted KNN model

5-fold CV (75	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 3.86

Global applicability domain: Inside

Local applicability domain index: 9.71e-01

Confidence level: 7.37e-01

Nearest Neighbors from the Training Set

Image not found

Tetrachloroethylene Measured: 3.48 Predicted: 3.86 Image not found

Butyl ether Measured: 3.89 Predicted: 3.93 Image not found

Nonene

Measured: 3.83 Predicted: 3.95

Image not found

Benzonitrile Measured: 4.46 Predicted: 3.95 Image not found

Ethylbenzene Measured: 3.74 Predicted: 3.87